Propargylamine

Other names:	2-Propyn-1-amine
	3-Amino-1-propyne
	2-Propynylamine
	3-Aminoprop-1-yne
	3-Aminopropyne
	1-Propine, 3-amino-
	Prop-2-ynylamine
	NSC 80642
Inchi:	InChI=1S/C3H5N/c1-2-3-4/h1H,3-4H2
InchiKey:	JKANAVGODYYCQF-UHFFFAOYSA-N
Formula:	C3H5N
SMILES:	C#CCN
Mol. weight [g/mol]:	55.08
CAS:	2450-71-7

Physical Properties

Property code	Value	Unit	Source
affp	887.40	kJ/mol	NIST Webbook
basg	853.50	kJ/mol	NIST Webbook
chl	-2100.80 ± 0.84	kJ/mol	NIST Webbook
gf	263.90	kJ/mol	Joback Method
hf	220.44	kJ/mol	Joback Method
hfl	206.00 ± 0.80	kJ/mol	NIST Webbook
hfus	11.70	kJ/mol	Joback Method
hvap	32.77	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	-0.422		Crippen Method
mcvol	54.510	ml/mol	McGowan Method
pc	5908.07	kPa	Joback Method
tb	355.00 ± 1.00	K	NIST Webbook
tb	356.20	K	NIST Webbook
tc	526.64	K	Joback Method
tf	253.80	K	Joback Method
vc	0.195	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	87.76	J/mol×K	330.69	Joback Method
cpg	92.73	J/mol×K	363.35	Joback Method
cpg	97.44	J/mol×K	396.01	Joback Method
cpg	101.91	J/mol×K	428.66	Joback Method
cpg	106.15	J/mol×K	461.32	Joback Method
cpg	110.17	J/mol×K	493.98	Joback Method
cpg	113.97	J/mol×K	526.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2450717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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